REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

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1. REPORT DATE *(DD-MM-YYYY)* 15-02-2011	2. REPORT TYPE Final Technical Report	3. DATES COVERED *(From - To)* From01-03-2008To31-11-2010

4. TITLE AND SUBTITLE

A Design Tool for Nanostructures with Tunable Thermal Properties

5a. CONTRACT NUMBER

5b. GRANT NUMBER
FA9550-08-1-0078

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force of Scientific Research
875 North Randolph Street
Arlington, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-OSR-VA-TR-2012-0217

12. DISTRIBUTION / AVAILABILITY STATEMENT

DIST. A

13. SUPPLEMENTARY NOTES

14. ABSTRACT

This research project is concerned with the development of novel nano-engineered materials whose thermal properties, such as thermal conductivity, can change in a predetermined manner due to internal and external triggers, such as temperature and mechanical stresses. The mechanisms that can dynamically change thermal properties of materials are dominated by submicron and nanoscale phenomena. In order to design systematically these materials, their submicron/nanoscale behavior needs to be modeled and predicted with sound accuracy but time and cost maneuverable. The PIs have developed a novel computational framework for the analysis and design of nano-structured materials with tunable thermal properties. This multiscale modeling approach is based on the Boltzmann transport equation (kinetic theory). Phonon transmission across dissimilar interfaces has been simulated with Nonequilibium Green's function approach. We have explored mechanical stress/strain as a mechanism for dynamically tuning thermal conductivity of materials. We have developed optical pump and soft X-ray nano-metrology for measuring nanoscale thermal transport. Our work made the first observation and quantitative measurement of non-Fourier heat dissipation from a nanoscale hot spot to the surroundings.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Ronggui Yang
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			**19b. TELEPHONE NUMBER** *(include area code)* 303-735-1003

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

A Design Tool for Nanostructures with Tunable Thermal Properties

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This research project is concerned with the development of novel nano-engineered materials whose thermal properties, such as thermal conductivity, can change in a predetermined manner due to internal and external triggers, such as temperature and mechanical stresses. The capability to control actively or passively the thermal properties of materials will allow for adapting dynamically the thermal transport paths to time varying operating conditions and enable radically improved thermal management systems, allowing for larger power densities in electronic components and larger operating temperatures of load barring structures as well as reducing thermally induced damage. The mechanisms that can dynamically change thermal properties of materials are dominated by submicron and nanoscale phenomena. In order to design systematically these materials, their submicron/nanoscale behavior needs to be modeled and predicted with sound accuracy but time and cost maneuverable.

With the AFOSR support, the PIs have developed a novel computational framework for the analysis and design of nano-structured materials with tunable thermal properties. The accomplishments of this 3-year project including:

1). A new multiscale modeling approach based on the Boltzmann transport equation (kinetic theory) for predicting phonon transport has been developed. This computational tool predicts adequately the thermal performance of the nanostructures balancing accuracy and turn-around time, and has been verified through comparison with standard Monte-Carlo simulation methods and experimental studies.

2). Frequency-dependent phonon transmission across interfaces of dissimilar materials has been simulated using the nonequilibium Green's function (NEGF) approach. Size-dependent phonon transmission has been studied for material interfaces with transverse or longitudinal confinements. This size-dependent phonon transmission is the key input parameter for the Boltzmann-equation based multiscale modeling tool for nanostructured materials.

3). We explored the dynamical tuning of Mthermal conductivity of materials using mechanical stress/strain. We have shown that strain effects on the lattice thermal conductivity of inorganic nanostructures and bulk polymer materials can be significant through molecular dynamics (MD) simulations.

4). An optical pump and soft X-ray probe measurement system has been developed to measure nanoscale thermal transport. Our work made the first observation and quantitative measurement of non-Fourier heat dissipation from a nanoscale hot spot to the surrounding, which was recently published in Nature Materials in 2010.

We have published 2 book chapters and 8 papers in high impact journals in 2008-2010 (1 in Nature Materials, 4 in Phys. Rev. B, 2 in J. Appl. Phys., 1 in Int. J. Num. Meth. Engr.). In addition, we currently have 3 journal papers accepted and 5 journal papers under review as of

February 2011. In addition, we have given about 30 invited and contributed presentations acknowledging the AFOSR support for this project.

In the following, we highlight the afore-mentioned achievements:

1). Multiscale Thermal Transport Modeling based on Boltzmann Transport Equation

Although the Boltzmann transport equation-based kinetic formulation is an attractive modeling and analysis approach for a widely applicable computational framework, solving the 7-dimension (3 in space, 2 in direction, 1 in frequency and 1 in time) integro-differential type Boltzmann equation is a prohibitively expensive and time-consuming task. Existing studies for phonon transport in nanoscale composites [1, 2, 3, 4] have several common assumptions that may not be appropriate: the shape of nanowires or nanoparticles in existing studies is regular, such as circular, rectangular or cubic, the size of the nanoparticles and nanowires is typically assumed to be uniform, and the distribution of these nano-inclusions is normally assumed to be periodic. Careful examination of the SEM images [Figure 1(a)] clearly shows that neither assumption is true for realistic nanocomposites. Extending either the discrete ordinate method or Monte Carlo simulation to more general nanostructures is not trivial. To analyze heat conduction at submicron scales of geometrically complex nano-structured materials, we have developed an extended finite element method (XFEM) is to solve the phonon Boltzmann transport equation as shown in Fig. 1(b) and (c) [5]. The geometry of the material interfaces is described by a level-set approach. Discontinuities of the phonon distribution across material interfaces are captured via enriched shape functions. To enforce interface scattering conditions and boundary conditions, a stabilized Lagrange multiplier method is used. The utility of the XFEM approach is demonstrated through the thermal analysis of experimentally characterized material samples [See Figure 1(c)]. The XFEM-BTE could potentially be extended to study thermoelectric and electrical properties of nanocomposites when electron BTE is solved along with the Poisson equation.
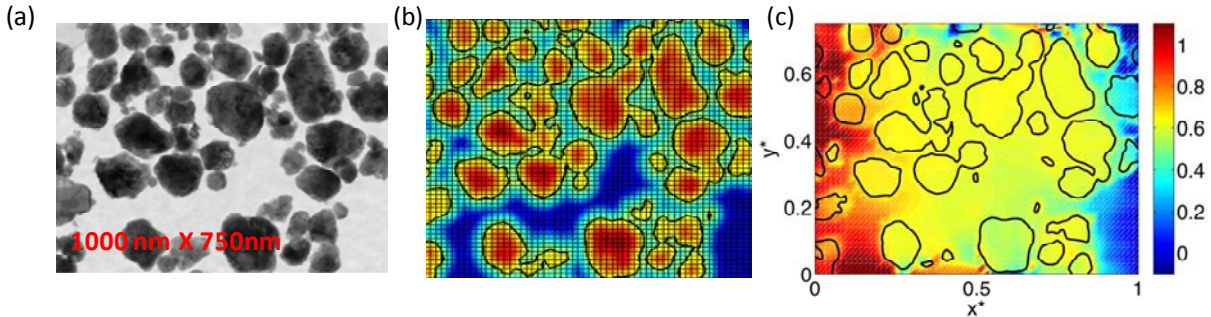

Figure 1. eXtended finite element method for phonon Boltzmann transport equation (XFEM-BTE) has been developed to study thermal conductivity of nano-enabled bulk materials with complex structures: (a). TEM image of the ball milled $Si_{80}Ge_{20}$ nanocomposites [6]. (b). Geometry described by level-set approach. (c). Temperature contours simulated with XFEM-BTE.

In general, a large number of acoustic and optical phonon distributions need to be simulated to accurate capture the dispersion characteristics of the individual material phases. In this project, a simpler and numerically less costly approach was pursued based on the single-distribution quasi-

static gray phonon model. Approximating the collision operator by a BGK approach, the governing equations of the gray phonon Boltzmann transport equation (GPBTE) are:

$$\mathbf{s} \cdot \nabla e = \frac{e^0 - e}{\Lambda} \qquad (\mathbf{x}, \boldsymbol{\mu}) \in \Omega \times S \qquad (1)$$

where the vector $\mathbf{s}$ denotes the propagation direction of the phonon; e is the phonon distribution, e^0 the equilibrium distribution and Λ the phonon mean free path length. Note the phonon distribution is defined as function of the spatial domain Ω and the velocity space S with $\mathbf{x}$ denoting the spatial and $\boldsymbol{\mu}$ the velocities coordinates.

Assuming an infinitely periodic material, the GPBTE, eqn. (1), is solved in a unit cell imposing proper periodic and symmetry boundary conditions. To capture phonon scattering at material interfaces, a diffusive mismatch model (DMM) has been adopted. More complex interface models can be easily integrated into the numerical framework developed in this project.

To represent the geometry of the material interfaces, a level-set presentation of the material layout is used. The level-set representation is reconstructed from a two-dimensional image of a material sample using standard image processing techniques. The material interface is defined by the zero level-set. To avoid the need for body-fitted meshes, an eXtended finite element approach (XFEM) has been adopted. This approach allows capturing the discontinuities at the material interfaces on structured meshes. A discontinuous Galerkin method has been identified as the method of choice for discretizing the velocity space.

XFEM has been originally developed for modeling crack propagation in solids which leads to a discontinuity in the displacements at the crack boundary. More recently XFEM has been applied to a broad range of problem involving discontinuous fields, such as phase change problems and multi-phase flows. In this project XFEM was adopted for solving the GPBTE with discontinuities in the phonon distributions along the material interfaces. In addition to the standard Galerkin approximation of the phonon distribution a discontinuous enrichment function is added:

$$e(\mathbf{x}, \boldsymbol{\mu}) = \sum_i N_i^{sp}(\mathbf{x}) \left[\hat{e}_i(\boldsymbol{\mu}) + \psi(\mathbf{x}) \, \hat{a}_i(\boldsymbol{\mu}) \right] \qquad (2)$$

where the $\psi(\mathbf{x})$ is the enrichment function and $\hat{a}_i(\boldsymbol{\mu})$ the associated unknown. To capture the discontinuity at the phonon interface, a Heaviside function is used to enrich the phonon distribution, i.e.

$$\psi(\mathbf{x}) = H(\mathbf{x}) = \begin{cases} +1 & \text{for} \quad x \in \Omega_I \\ 0 & \text{for} \quad x \in \Omega_{II} \end{cases} \qquad (3)$$

Note the enrichment is only active in elements intersected by a material interface, i.e. the unknown $\hat{a}_i(\boldsymbol{\mu})$ is set to zero in all elements that are not intersected or adjacent to an intersected element.

The approximation (2) is used to discretize in space the weak form of the governing equations (1). As the problem is convection dominant, the discretized problem suffers from numerical instabilities and needs to be stabilized. In this project a Streamline-Upwind Petrov-Galerkin (SUPG) stabilization approach is used. In the context of GPBTE the numerical diffusion introduced by SUPG can be well controlled and leads to minor additional computational cost.

To enforce the interface conditions of the DMM a stabilized Lagrange multiplier formulation was developed. To satisfy the inf-sup stability condition for mixed finite element formulations, it is usually sufficient to select the approximation space for the Lagrange multipliers to be one

polynomial order lower than the space for the physical field, i.e. the phonon distribution. To overcome the additional complexity due the stabilized Lagrange multiplier formulation, a much simpler phonon-flux interface condition was recently developed. This formulation is derived via integration by parts the weak form of the governing equations (1). For example for phase I, this leads to:

$$\int_\Omega \delta e\left[s\cdot\nabla e + \frac{1}{\Lambda}\left(e^I - e^{I0}\right)\right]d\Omega = \int_\Gamma \delta e\, s\cdot n\, e^I\, d\Gamma - \int_\Omega \delta\nabla e\cdot s\, e^I\, d\Omega + \int_\Omega \delta e\,\frac{1}{\Lambda}\left(e^I - e^{I0}\right)d\Omega$$

(4)

The boundary term allows satisfying the DMM conditions without Lagrange multipliers by substituting the incoming fluxes with the DMM condition (2) as follows:

$$\int_\Gamma \delta e\, s\cdot n\, e^I\, d\Gamma = \int_{s\cdot n>0} \delta e\, s\cdot n\, e^I\, d\Gamma + \int_{s\cdot n<0} \delta e\, s\cdot n\, \tilde{e}^I\, d\Gamma$$

(5)

with

$$\tilde{e}^I = \frac{-\alpha_{12}\displaystyle\int_{s\cdot n>0}\mathbf{s}\cdot\mathbf{n}\,e^I\,d\mu + \alpha_{21}\displaystyle\int_{s\cdot n<0}\mathbf{s}\cdot\mathbf{n}\,e^{II}\,d\mu}{\displaystyle\int_{s\cdot n<0}\mathbf{s}\cdot\mathbf{n}\,d\mu}$$

In this project, the XFEM formulation of the GPBTE was studied extensively for a discrete ordinate discretization of the velocity space. Reference results were taken from the square-inclusion example of Chen and Yang [7] (see figure 2). Additional problems using real samples of nano-composites were studied. Numerical studies suggested that the XFEM formulation features the same accuracy and stability as finite element and finite volume formulation requiring body-fitted meshes. Comparison between XFEM predictions and experimentally measured heat conductivities from Joshi et al. 2008 showed good agreement [see Figure 1].
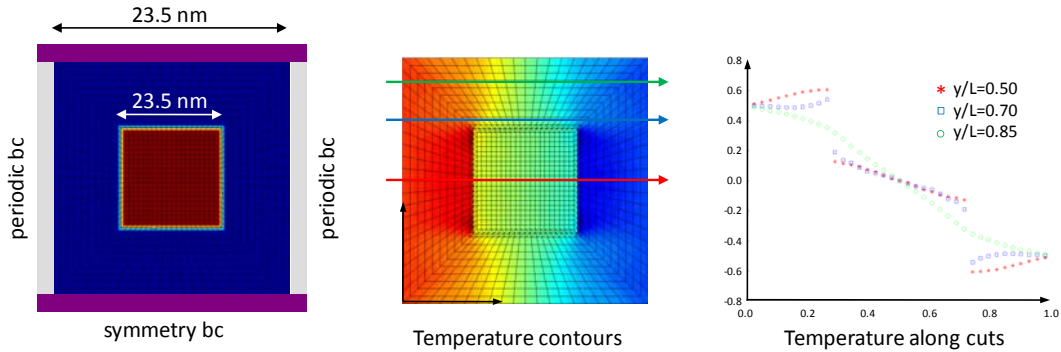

Figure 2: XFEM Analysis of synthetic nano-composite with Si square inclusions in a Ge host [2].

However, a significant limitation of our current XFEM-BTE is that we used the acoustic mismatch model (AMM) [8], and diffuse mismatch model (DMM) [8] for phonon transmission across material interfaces, which are standard practice today by various groups but are indeed incorrect for realistic material interfaces.

2 Phonon Transmission across Coherent Interfaces

Realizing that carrier transport across interfaces is the key to the superior properties of nano-enabled bulk materials and the currently available AMM and DMM model could not be valid in realistic materials, we have investigated a variety of modeling approaches for phonon

transmission across interfaces. Molecular dynamics simulation has been used extensively to study the interface thermal resistances of various materials. However, the results could only be used to qualitatively understand the impact of interfaces, but not useful for qualitative design, since it cannot be scaled up or integrated into a multiscale simulation tools.

The multiscale BTE solvers described in session 1) essentially need frequency-dependent phonon transmission or energy-dependent electron transmission across interfaces as input parameters. For phonon transmission across interfaces, atomistic methods such as phonon wave-packet method [9], linear lattice dynamics approach [10] and nonequilibrium Green's function (NEGF) approach [11-20] has recently been developed. Among these atomistic methods, NEGF is the most efficient one for calculating phonon transmission across interfaces for considering detailed atomic micro-structures. The NEGF approach calculates phonon transmission by solving the lattice dynamics equation under harmonic approximation using the Green's function method.

Under harmonic approximation, the dynamical equation of a lattice system can be solved with the Green's function method,

$$(\omega^2 \mathbf{I} - H)G = \mathbf{I}, \qquad (6),$$

where H is the dynamical matrix and G is the Green's function. The Green's function represents the response of the system to an infinitesimal perturbation. For a general interface system which consists reservoirs 1 and 2, and an interface region as shown in Figure 3, the total phonon transmission across the interface region can be formulated as,
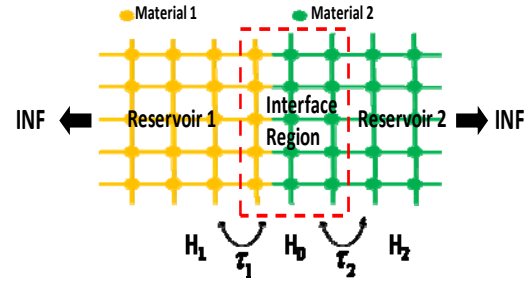

Figure 3. A general interface system for phonon transmission calculation using NEGF approach. The system is generally divided into three parts: reservoir 1, interface region and reservoir 2. H is the dynamical matrix of each part and τ represents the interactions between the reservoirs and the interface region.

$$\Xi(\omega) = Trace[\Gamma_1 G_{D,D} \Gamma_2 G_{D,D}^+], \qquad (7),$$

where $G_{D,D}$ is the Green's function of the interface region solved from equation (6) and $\Gamma_{1,2}$ are related to the self-energy matrices due to the coupling between the reservoirs and the interface region, which can be calculated from dynamic matrix $H_{1,2}$ and the interaction $\tau_{1,2}$.

The transmission function at each particular phonon frequency can be written as,

$$t(\omega) = \Xi(\omega) / \Xi(\omega)_{Reservoir1}, \qquad (8),$$

where $\Xi(\omega)_{Reservoir1}$ is the total phonon transmission in pure materials 1.

The above NEGF method is a general method and can be applied to any atomistic system under harmonic approximation. However the application of this method can be greatly limited due to the challenge of solving equation (6) if the system size is too large. To make the matrix system solvable, the studies so far using NEGF usually assume that the atomistic system is lattice matched (coherent interface with same lattice constants). A number of systems have been studied with NEGF approach, such as low dimensional molecular chains, coated nanowires, amide-linked nanotubes and lattice matched Si/Ge, etc.

Figure 4 shows our recent studies [X.B. Li, et. al., Submitted to PRB]. Figure 4(a) shows that phonon transmission across Si-Ge interface (assuming same lattice constant of the two materials) calculated using NEGF agrees well with the one obtained from lattice dynamics [10]. Figure 4(b) shows phonon transmission across Si/Ge like materials interface by varying the mass in Ge-like

material while keeping the Ge force filed. With varying mass ratio phonon dispersion mismatch can be tuned and significant change can be obtained for phonon transmission. Figure 4(c) shows the thermal conductance across the Si/Ge like materials interface and an optimal mass ratio at 1.26 exists for achieving the maximum thermal conductance.
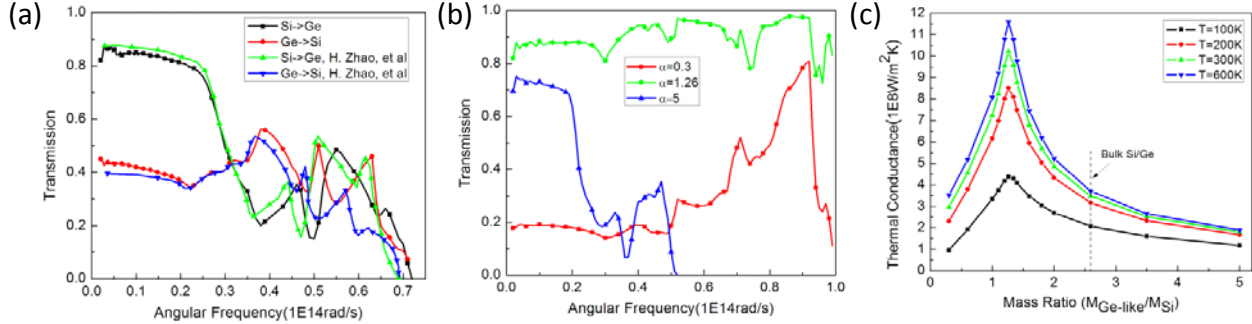

Figure 4. (a) Phonon transmission across lattice matched Si-Ge interface using NEGF. The results agree well with lattice dynamics calculations. (b) phonon transmission across $S(M_1)/Ge$ like(M_3) interfaces with varying mass ratio: $\alpha = M_3 / M_1$. (c) Thermal conductance across the interface as a function of the mass ratio.

However, the current NEGF approach has assumed lattice-matched systems and harmonic approximations, which greatly limits the power of NEGF approach. For example, strain effects on phonon transmission has been studied for the lattice matched Si/Ge interface [14] and the results only show very small difference from the unstrained interface, which does not agree with experimental results [21]. This suggests the importance of considering the realistic material interfaces (with lattice mismatch). The anharmonic effects have also been addressed in several studies; however the method has only been applied to simple one-dimensional chains due to the computational complexity. Further developments need to be focused on addressing these challenges in realistic material interfaces.

3. Tuning Thermal Conductivity of Materials using mechanical Stress/Strain.

Different methods can be used for tune thermal conductivity of materials. Among these methods, mechanical strain provides an efficient way. We have performed molecular dynamics (MD) simulation to systematically study the strain effects on the lattice thermal conductivity of inorganic materials (mainly nanostructures: Si nanowire and thin film, single-walled carbon naotube (SWCNT) and single layer graphene) and bulk polymer materials [X.B. Li, et. al., PRB (2010), J. Liu, et. al., PRB (2010)]. Results show that thermal conductivity of the strained silicon nanowires and thin films decreases continuously when the strain changes from compressive to tensile. However, the thermal conductivity has a peak value under compressive strain for SWCNT and at zero strain for single layer grapheme as shown in Fig. 5(a) for results on SWCNT. In contrast, thermal conductivity of polymer materials increases with increasing tensile strain as shown in Fig. 5(b). The underlying mechanisms are analyzed in this paper for both types of materials. We found that the thermal conductivity of inorganic materials can be related to the phonon dispersion curve change and structural buckling under strain and for polymer chains thermal conductivity directly connects to the orientations of the chains instead of strain rates. This thermal conductivity dependence with strain can guide us to tune the thermal conductivity for materials in applications.
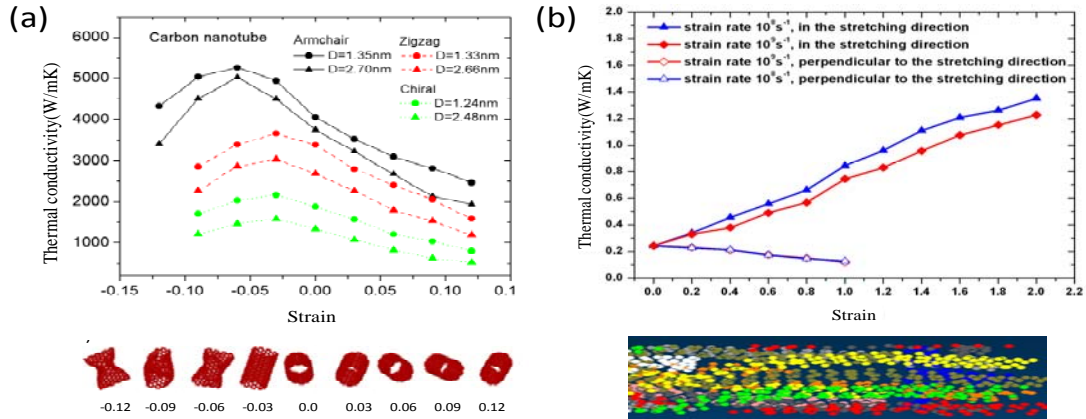
Figure 5. (a). Strain effects on the lattice thermal conductivity of armchair, zigzag and chiral SWCNTs. (b). Strain effects on bulk polymer materials. Different strain effects are observed for these two kinds of materials.

4. Characterizing Nanoscale Thermal Transport using Soft X-Ray Probes

Femtosecond laser is a unique tool to study a number of ultrafast relaxation processes and nanoscale transport phenomena. Fourier theory of heat conduction considers heat transport as a diffusive process where energy flow is driven by a temperature gradient. However, at length scales smaller than the mean free path for the energy carriers, heat flow becomes ballistic - driven by direct point-to-point transport of energy quanta. Although past experiments have seen ballistic effects in layered thin films or nanowires, non-Fourier heat dissipation from a nanoscale hot spot to the surrounding had not been experimentally observed and was a subject of some uncertainty although it has significant relevance in heat dissipation of electronic transistors. Our work made the first observation and quantitative measurement of this geometry using the excitation and detection scheme shown in Fig. 6 in exciting recent work recently published in Nature Materials in 2010 [M. Siemens, et. al, Nature Materials (2010)]. We use a beam of ultrafast coherent soft x-rays, at a wavelength of 29 nm, to directly observe the cooling dynamics of a nanoscale heat source into its bulk surroundings. By interferometrically monitoring displacement in a heated nanostructure using diffraction of soft x-ray light, we can detect dynamic temperature changes more sensitively than would be possible using either ultrashort optical pulse probing or steady-state measurements. This ultrafast short-wavelength transient diffraction methodology represents a newly-developed experimental capability that allows us to map out nanoscale thermal transport over a range of nanostructure sizes.

SUMMARY

To close, we have made significant progresses over the past 3 years for the development of nanostructured materials with tunable thermal properties. We have developed a novel computational framework for the analysis and design of nano-structured materials with tunable thermal properties. This novel multiscale modeling approach is based on the Boltzmann transport equation (kinetic theory). We have developed nonequilibrium Green's function approach for studying phonon transmission across interfaces of dissimilar materials. Mechanical stress has been explored as a mechanism for tuning thermal conductivity of materials. We have also developed optical pump soft X-ray probe based nano-scale metrology for measuring nanoscale thermal transport. Our work made the first time observation and quantitative measurement of

non-Fourier heat dissipation from a nanoscale hot spot to the surroundings. We have also identified future research directions for the development of nanostructured materials with tunable thermal properties.
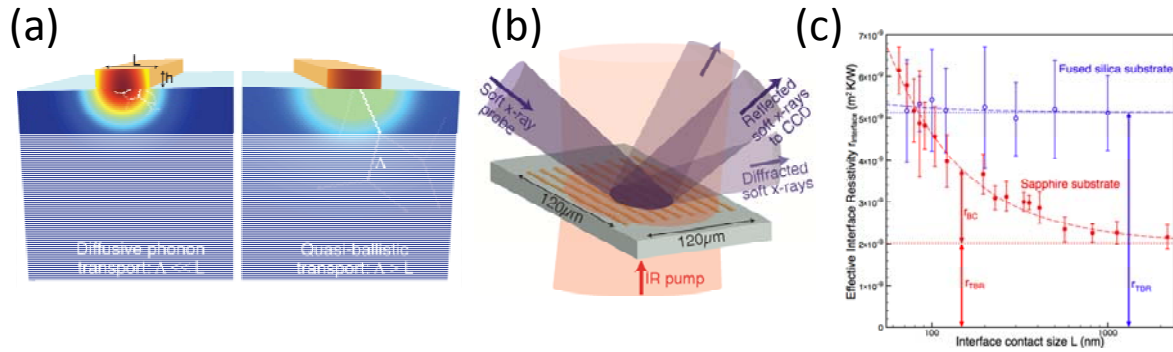

Figure 6: (a) Schematic illustrating the difference between diffusive and quasi-ballistic thermal transport across a nano-interface. (b) Sample geometry showing laser heating and EUV detection of heat flow from nanostructures to the bulk substrate underneath. (c) Measured thermal resistivity from Ni nanostructures to fused silica (blue) or sapphire (red) substrates. The blue and red dashed curves show model predictions for the ballistic resistivity correction, assuming phonon mean free paths of 2nm (FS) and 120nm (sapphire). For linewidths< 200nm on sapphire, heat flow into the bulk is significantly slower than predicted by the Fourier Law.

Awards Received by the PI in 2008-2010

2010 ASME Bergles-Rohsenow Young Investigator Award in Heat Transfer (Citation for this award: For developing modeling and experimental tools to understand micro/nanoscale thermal transport and for innovative applications of micro/nano-structure in macroscale forms for energy conversion and thermal management.)

2010 Dean's Award for the Outstanding Junior Faculty Member, College of Engineering and Applied Science, University of Colorado

2010 Biography featured as a technology developer with outstanding potential that could reverse the decline in the book "The Rise and Fall of American Technology" by Dr. Lynn G. Gref.

2009 Selected as one of the 88 Invited Participants, the US National Academy of Engineering's (NAE) 15th U.S. Frontiers of Engineering Symposium.

2008 Technology Review's TR35 Award (one of the 35 young scientists and technologists in world who are under the age of 35, but their work--spanning medicine, computing, communications, electronics, nanotechnology, energy, and more--is changing our world.)

2008-2011 Sanders Faculty Fellow, College of Engineering and Applied Science, CU-Boulder.

2008 Outstanding Research Award, Department of Mechanical Engineering, CU-Boulder

Journal Publications and Book Chapters

Book Chapters

1. Suraj J. Thiagarajan, Wei Wang, and Ronggui Yang, "Nanocomposites as High Efficiency Thermoelectric Materials," in Annual Review of Nano Research, Volume 3, ed. G.Z. Cao, Q.F. Zhang, and C.J. Brinker, World Scientific Publisher Co., Singapore, p. 447-492, 2009.

2. Pilhwa Lee, Kurt Maute and Ronggui Yang, 'An Extended Finite Element Method for the Analysis of Submicron Heat Transfer Phenomena," book chapter in "Multiscale Methods in Computational Mechanics" in the Springer series ["Lecture Notes in Applied and Computational Mechanics](#)", to appear in October 2010.

Journal Papers Published
(1 in Nature Materials, 4 in Phys. Rev. B, 2 in J. Appl. Phys., 1 in Int. J. Num. Meth. Engr.)

1. Mark Siemens, Qing Li, Ronggui Yang, Keith A. Nelson, Eric Anderson, Margaret Murnane, and Henry Kapteyn, Quasi-ballistic thermal transport from nanoscale interfaces observed using ultrafast coherent soft X-ray beams, Nature Materials, Vol. 9, pp. 26-30, 2010

2. Jun Liu and Ronggui Yang, Tuning the Thermal Conductivity of Polymers with Mechanical Strain, Physical Review B, 81, Art # 174122, 2010

3. Xiaobo Li, Kurt Maute, Martin L. Dunn and Ronggui Yang, Strain Effects on the Thermal Conductivity of Nanostructures, Physical Review B, 81, Art #245318, 2010.

4. Jun Zhou, and Ronggui Yang, Thermoelectric Transport in Strongly Correlated Quantum Dot Nanocomposites, Submitted to Physical Review B, 82, 075324, 2010.

5. Jun Zhou, Xiaobo Li, Ronggui Yang, and Gang Chen, A Semi-Classical Model for Thermoelectric Nanocomposites, Physical Review B, Vol. 82, Art #. 115308,

6. Jie Zhu, Dawei Tang, Wei Wang, Jun Liu, Kristopher W Holub, and Ronggui Yang, Ultrafast Thermoreflectance Techniques for Measuring Thermal Conductivity and Interface Thermal Conductance of Thin Films, Journal of Applied Physics, 108, Art # 094315, 2010

7. Liang-Chun Liu, Mei-Jiau Huang, Ronggui Yang, Ming-Shan Jeng, and Chang-Chung Yang, Curvature Effect on the Phonon Thermal Conductivity Reduction of Dielectric Nanowires, Journal of Applied Physics, Vol. 105, n10, Art # 104313, May 2009.

8. Evgrafov, K. Maute, R.G. Yang, and M.L. Dunn, Topology Optimization for Nano-scale Heat Transfer (Published online in July 2008), International Journal for Numerical Methods in Engineering, Vol. 77, pp. 285–300, 2009

Journal Papers Accepted and Submitted

1. Jose Ordonez-Miranda, Ronggui Yang, and J.J. Alvarado-Gil, A New Constitutive Equation for Nano-to-Macro- Scale Heat Conduction Based on Boltzmann Transport Equation, Journal of Applied Physics, Accepted.

2. Jose Ordonez-Miranda, Ronggui Yang, and J.J. Alvarado-Gil, The Effect of the Electron-Phonon Coupling on the Effective Thermal Conductivity of Metal-Nonmental Multilayers, Journal of Applied Physics, Accepted.

3. Jun Zhou, and Ronggui Yang, Quantum and Classical Thermoelectric Transport in Nanocomposites, Physical Review B, Accepted.

4. Xiaobo Li, and Ronggui Yang, Size-Dependent Phonon Transmission across Interfaces of Dissimilar Materials, Submitted to Physical Review B, Submitted.

5. David Makhija, Ronggui Yang, and Kurt Maute, A Comparative Study of Velocity Discretization Schemes for the Phonon Boltzmann Transport Equation, Numerical Heat Transfer, Submitted.
6. Kurt Maute, Sebastain Kreissl, Ronggui Yang, and David Makhija, Topology Optimization of Heat Conduction in Nanocomposites, Structural and Multidisciplinary Optimization, Submitted.
7. David Makhija, Georg Pingen, Ronggui Yang, and Kurt Maute, Topology Optimization of Multi-component flows by Multi-relaxation Time Lattice Boltzmann Method, Structural and Multidisciplinary Optimization, Submitted.
8. Jose Ordonez-Miranda, Ronggui Yang, and J.J. Alvarado-Gil, A Model for the Effective Thermal Conductivity of Metal-Nonmetal Nanocomposites, Physical Review B, Submitted.

Invited Conference Presentations

1. Mark Siemens, Qing Li, Margaret Murnane, Henry Kapteyn, Ronggui Yang, Probing Nanoscale Thermal Transport using Extreme Ultraviolet (EUV), SPIE Photonics West '11 Conference, San Francisco, California, January 22-27, 2011.
2. Ronggui Yang, US-Japan Seminar on Nanoscale Thermal Transport, Izu, Japan, June 26-29, 2011.
3. Ronggui Yang, Scaling Up Nanoscale Effects in Thermal Transport for Thermoelectricity and Thermal Management, InterAgency Power Group Meeting (Air Force, Army, Navy, Department of Energy, and NASA), Golden, CO, May 3-7, 2010.
4. Ronggui Yang, Micro/Nano-enabled High Heat Flux Devices, DARPA/DSRC Physics of High Heat Flux Devices and their Applications Workshop, Arlington, VA, November 11-12, 2009
5. Ronggui Yang, "Energy Transport at Nanoscale: Modeling, Characterization and Applications." Thin Air Philosophical Society (TAPS) Symposium on "Current Challenges in Mechanics and Materials" Boulder, CO, August 3-6, 2010.
6. Invited: Kurt Maute, Pilhwa Lee, Georg Pingen, and Ronggui Yang, Design Optimization of Transport Phenomena at Micro and Submicron Scale via Kinetic Theory Approaches, Conference on Multi-scale Modeling in Computational Mechanics, Rolduc, The Netherlands, March 11-13 2009
7. Ronggui Yang, Thermoelectric Nanocomposites: A Cheaper Nanotech Solution to Cleaner and Quieter Global Energy, EmTech 2008 organized by MIT Technology Review, September 23-25, MIT campus, MA.
8. Ronggui Yang, et al, Probing Nanoscale Thermal Transport using Extreme Ultraviolet (EUV) Light, 6th Japan- US Joint Seminar on Nanoscale Transport Phenomena - Science and Engineering," July 13-16, 2008, Radisson Hotel, Boston, MA.
9. Xiaochun Wang, Ronggui Yang, Yong Zhang, Jean-Pierre Fleurial, Andrew F. May, and G. Jeffrey Snyder, First Principles Study on Thermoelectric Properties of Lanthanum Chalcogenides, 6th Japan- US Joint Seminar on Nanoscale Transport Phenomena - Science and Engineering," July 13-16, 2008, Radisson Hotel, Boston, MA.

Invited Seminars

1. February 8, Thermal Science and Engineering for Thermoelectric Energy Conversion, Department of mechanical Science and Engineering, University of Illinois, Urbana-Champaign, IL.
2. December 3, 2010, Scalable Thermal Management Technologies: from Atoms to Systems, Department of Mechanical Engineering, MIT, Cambridge, MA.
3. March 24, 2010, Nano-Enabled Energy Conversion and Thermal Management: from Fundamental Sciences to Manufacturable Systems, Department of Mechanical and Aerospace Engineering, Rutgers University, New Brunswick, NJ.
4. March 22, 2010, Nano-structured Thermal Interfaces for Sustainable Energy technologies, Department of Mechanical and Nuclear Engineering, Pennsylvania State University, University Park, PA.
5. February 25, 2010, Nano-structured Thermal Interfaces for Sustainable Energy technologies, Mechanical Engineering, California Institute of Technology, Pasadena, CA.
6. February 24, 2010, Nano-structured Thermal Interfaces for Sustainable Energy technologies, Department of Mechanical Engineering and Materials Sciences, Duke University, NC.
7. November 23, 2009, Nano-Enabled Energy Conversion and Thermal Management: from Fundamental Sciences to Manufacturable Systems, Department of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland OH.
8. June 2, 2009, Challenges and Opportunities in Nanoscale Heat Transfer, Department of Physics, Xiamen University.
9. June 1, 2009, Challenges and Opportunities in Nanoscale Heat Transfer, Department of Electrical and Information Engineering, Putian University.
10. June 26, 2008, Nanoscale Heat Transfer: Challenges and Opportunities, National Renewable Energy Lab, Golden, CO [Host: Dr. Sreekant Narumanchi and Dr. Kenneth Kelly].

REFERENCES

1 Weixue Tian and Ronggui Yang, Effect of Interface Scattering on Phonon Thermal Conductivity Percolation in Random Nanowire Composites, Applied Physics Letters 90, 263105, June 2007,

2 Ming-Shan Jeng, Ronggui Yang, David W. Song, and Gang Chen, Modeling the Thermal Conductivity and Phonon Transport in Nanoparticle Composites using Monte Carlo Simulation, ASME Journal of Heat Transfer, Vol. 130, Article #042410 (1-11), April 2008

3 Mazumder, S., and Majumdar, A., 2001, "Monte Carlo study of phonon transport in solid thin films including dispersion and polarization," J. Heat Trans. 123(4):749-759.

4 Lacroix, D., Joulain, K., and Lemonnier, D., 2005, "Monte Carlo transient phonon transport in silicon and germanium at nanoscales," Phys. Rev. B 72, Art No. 064305.

5 Pilhwa Lee, Ronggui Yang and Kurt Maute, "An Extended Finite Element Method for the Analysis of Submicron Heat Transfer Phenomena," in "Multiscale Methods in Computational Mechanics", Nov. 2010.

6 Giri Joshi, Hohyun Lee, Yucheng Lan, Xiaowei Wang, Gaohua Zhu, Dezhi Wang, Ryan W. Gould, Diana C. Cuff, Ming Y. Tang, Mildred S. Dresselhaus, Gang Chen, Zhifeng Ren, "Enhanced Thermoelectric Figure-of-Merit in Nanostructured p-type Silicon Germanium Bulk Alloys," Nano Letters 2008 8 (12), 4670-4674

7 Ronggui Yang and Gang Chen, Thermal Conductivity Modeling of Periodic Two-Dimensional Nanocomposites, Physical Review B, Vol. **69**, 195316 (1-10), 2004

8 E. T. Swartz and R. O. Pohl, "Thermal boundary resistance," Rev. Mod. Phys. 61, 605 (1989).

9 P.K. Schelling, S.R. Phillpot, and P. Keblinski, "Phonon wave-packet dynamics at semiconductor interfaces by molecular-dynamics simulation," Appl. Phys. Lett. 80, 2484 (2002)

10 H. Zhao and J. B. Freund, "Lattice-dynamical calculation of phonon scattering at ideal Si-Ge interfaces," J. Appl. Phys. 97, 024903 (2005).

11 W. Zhang, T. S. Fisher, and N. Mingo, "The atomistic Green's function method: an efficient simulation approach for nanoscale phonon transport", Numerical heat transfer 51, 333, 2007.

12 N. Mingo, "Anharmonic phonon flow through molecular-size junctions," Phys. Rev. B 74, 125402 (2006).

13 N. Mingo and Liu Yang, "Phonon transport in nanowires coated with an amorphous materials: an atomistic Green's function approach," Phys. Rev. B 68, 245406 (2003).

14 W. Zhang, T.S. Fisher and N. Mingo, "Simulation of interfacial phonon transport in Si-Ge heterostructures using an atomistic Green's function method," J. Heat Transfer, 129, pp. 483-491 (2007).

15 J.-S. Wang, N. Zeng, J. Wang, and C. K. Gan, "Nonequilibrium Green's function method for thermal transport in junctions," Phys. Rev. E 75, 061128 (2007)

16 Y. Xu, J.-S. Wang, W. Duan, B.-L. Gu, and B. Li, "Nonequilibrium Green's function method for phonon-phonon interactions and ballistic-diffusive thermal transport," Phys. Rev. B 78, 224303 (2008).

17 J.-S. Wang, J. Wang, and N. Zeng, "Nonequilibrium Green's function approach to mesoscopic thermal transport," Phys. Rev. B 74, 033408 (2006).

18 J. Wang and J.-S. Wang, "Dimensional crossover of thermal conductance in nanowires," Appl. Phys. Lett. 90, 241908 (2007).

19 J. T. Lu and J.-S. Wang, "Quantum phonon transport of molecular junctions amide-linked with carbon nanotubes: a first-principle study," Phys. Rev. B 78, 235436 (2008)

20 T. Yamamoto and K. Watanabe, "Nonequilibrium Green's function approach to phonon transport in defective carbon nanotubes," Phys. Rev. Lett. 96, 255503 (2006)

21 J. Q. He, J. R. Sootsman, S. N. Girard, J.-C. Zheng, J. G. Wen, Y. M. Zhu, M. G. Kanatzidis and V. P. Dravid, "On the Origin of Increased Phonon Scattering in Nanostructured PbTe Based Thermoelectric Materials," Journal of the American Chemical Society, 132 (25), 8669-8675 (2010)